ACCURATE PREDICTION OF THERMODYNAMIC PROPERTIES OF ALCOHOLES, KETONES AND ETHERS BY MCORGC EOS

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Abstract   This paper presents the ability of a new group contribution equation of state in the prediction of thermodynamic properties of alcoholes, ketones and ethers. This equation of state, called MCORGC, is based on the Chain-Of-Rotators Group Contribution equation considering a NRTL type local composition mixing rule. The group parameters required to predict the thermodynamic properties of the oxygenated compounds are reported. In order to test the accuracy of the new proposed equation of state, saturated thermodynamic properties of several alcoholes, ketones and ethers are predicted over a wide range of pressures and temperatures and compared with the values reported in the literature. In addition, the capabilities of MCORGC have been compared with other equations of state.

Key Words   Theory, Equation of State, Group Contribution, Polar, Nonpolar, Alcoholes, Ketones, Ethers

چکیده   این مقاله توانایی یک معادله حالت مشارکت گروهی جدید در انجام پیش‌بینی خواص ترمودینامیکی الکل‌ها، ستون‌ها و اترها را ارائه می‌دهد. نام این معادله MCORGC می‌باشد و بر اساس زنجیره چرخان و مشارکت گروهی و با استفاده از قوانین اختلاط موضعی NRTL عمل می‌کند. پارامترهای مورد نیاز محاسبه خواص ترمودینامیکی اجسام اکسیژن دار، گزارش شده است. جهت آزمایش دقت این معادله حالت، خواص چندین الکل، ستون و اتر محاسبه شده و با اطلاعات تجربی در شرایط متفاوت مقایسه شده است. بعلاوه دقت این معادله حالت با چندین معادله دیگر مقایسه شده است.

INTRODUCTION

Thermodynamic properties of pure and multicomponent systems play an important role in simulation and design of separation processes and transmission pipelines. Therefore, an accurate prediction of thermodynamic properties is highly desirable in chemical industries. The number of systems of interest to the chemical industries is enormous even when the scope of components is restricted to low molecular mass (e.g. a carbon number less than 25). Hence, it is desirable to be able to predict phase equilibrium based on as little experimental information as possible or at best without any experimental data at all.

The equations of state have been a practical tool for predicting thermodynamic properties of pure and mixed components. The equations of state like SRK and PR have been developed for nonpolar components in gas phase and then generalized to liquid phase and slightly polar components. Prediction of thermodynamic properties of liquid phase by equations of state can be improved by using activity coefficient equations based on the gorup contribution models. Some of the well-known equations of this kind are NRTL and UNIFAC. The new generation of equations of state has been developed by combination of both group contribution and free volume models. These kinds of equations of state are more accurate in predicting both gas and liquid, polar and nonpolar

systems. PFGC (Cunnigham, 1974, Moshfeghian et al. 1980, and Moshfeghian, 1989), GC-EOS (Jorgensen, 1984) and CORGC (Pults and Chao 1988 and Shariat et al. 1993) are members of this generation of equations of state. The main advantage of group contribution equations of state is the fact that they don't require any critical properties, because these properties for fluids such as heavy fraction in gas condensate, crude oils or coal derived compounds are not readily available or if they exist they are not accurate enough to rely upon.

The CORGC has been introduced by Pults and Chao (1988) with limited applications. Recently, Shariat et al. (1993) revised the parameters of CORGC and extended its application to polar and halogenated systems. The MCORGC is the latest group contribution equation of state developed by Zia-Razzaz and Moshfeghian (1993). In order to improve the accuracy of CORGC, they applied a new local composition model and combined it with CORGC. They reported parameters for 37 groups and showed the promising capabilities of this equation in predicting thermodynamic properties for pure and mixture, as well as for polar and nonpolar systems.

In continuation of our previous study, this paper focuses on the ability of MCORGC in prediction of thermodynamic properties of the oxygenated compounds which have found a great deal of applications in industry, specifically in the field of oxygenated fuels.

THE MCORGC EQUATIONS

Zia-Razzaz and Moshfeghian (1993) have proposed their equation of state as a summation of the attractive and repulsive contributions in the form of:

$$Z = \frac{1+y+y^2-y^3}{(1-y)^3} + [\frac{c(\alpha-1)}{2}][\frac{3y+3\alpha y^2-(\alpha+1)y^3}{(1-y)^3}]$$
$$- \frac{a}{RT(V+b)} + \frac{a^*V}{b}\log(1+\frac{b}{V})$$ (1)

The following mixing rules are used in the proposed equation. In these relations the parameters b_m, c_m and q_m are used for the group and b, c and Q for the fluid covolume, equivalent degree of freedom and the normalized area, respectively.

$$b = \sum_i^{NC} x_i \sum_m^{NG} v_{im} b_m$$ (2)

$$C = \sum_i^{NC} x_i \sum_m^{NG} v_{im} C_m$$ (3)

$$Q = \sum_i^{NC} x_i \sum_m^{NG} v_{im} q_m$$ (4)

$$\theta_m = \frac{\sum_i^{NC} x_i v_{im} q_m}{Q}$$ (5)

$$y = \frac{b}{4V}$$ (6)

$$\tau_{mn} = \exp[\frac{a_{mn}(a_{mn}-a_{nn})}{RTQV}]$$ (7)

$$a = \frac{Q^2 \sum_m^{NG} \sum_n^{NG} \theta_m \theta_n a_{mn} \tau_{mn}}{\sum_l^{NG} \theta_l \tau_{ml}}$$ (8)

$$a^* = (\partial a/\partial V)_{T,n} = RTQ \sum_m^{NG} \theta_m (H2_m H6_m - H5_m)$$ (9)

The parameters b_m and a_{mn} are temperature dependent and their temperature dependency is

$$b_m = b_m^* \exp(-\frac{T}{T_m^*})$$ (10)

$$a_{mn} = a_{mn}^* (\frac{T}{T_{mn}^*})^{-0.18135} \exp(-\frac{T}{T_{mn}^*})$$ (11)

where b_m^*, T_m^* are group parameters and a_{mn}^* and T_{mn}^* are the attraction parameter and the characteristic temperature, respectively.

Based on Equation 1, other termodynamic properties such as fugacity coefficient ϕ_i, entropy departure S^R, and enthalpy departure H^R can be derived from fundamental thermodynamic relations. The resulting expression for fugacity coefficient is:

$$\ln \phi_i = \frac{4y - 3y^2}{(1-y)^2} + \frac{C_i(\alpha-1)}{2}\{\frac{(4+\alpha)y - 3y^2}{(1-y)^2} + (1+a)$$

$$\ln(1-y)\} - \frac{ab_i}{RTb(v+b)} - \frac{b_i}{b}\{\frac{1+y+y^2-y^3}{(1-y)^3}$$

$$+ \frac{C(\alpha-1)[3y + 3\alpha y^2 - (\alpha+1)y^3}{2(1-y)^3}\} + (A_i + \frac{ab_i}{b})$$

$$\ln(1+4y) - \ln Z \tag{12}$$

where

$$A_i = [\frac{\partial(n^2 a)}{\partial n_i}]_{T,V,n_j} \tag{13}$$

$$A_i = -RTV \sum_m^{NG} v_{im}q_m H2_m + \theta_m \{Q_i[H5_m + H2_m(1-H6_m)]\cdot$$

$$+ H3_{im} - H2_m H7_{im}\} \tag{14}$$

$$b_i = \sum_m^{NG} v_{im} b_m \tag{15}$$

$$C_i = \sum_m^{NG} v_{im} C_m \tag{16}$$

$$Q_i = \sum_m^{NG} v_{im} q_m \tag{17}$$

$$H2_m = \sum_k^{NG} \theta_k \tau_{km} a_{km}(Q/RTV)/H4_m \tag{18}$$

$$H3_{im} = \sum_k^{NG} q_k v_{ik} a_{km}(Q/RTV)/H4_m \tag{19}$$

$$H4_m = \sum_k^{NG} \theta_m \tau_{km} \tag{20}$$

$$H5_m = \sum_k^{NG} \theta_k \tau_{km} a_{km}(a_{km} - a_{mm}) \alpha_{km}(Q/RTV)^2/H4_m \tag{21}$$

$$H6_m = \sum_k^{NG} \theta_k \tau_{km} a_{km}(a_{km} - a_{mm})(Q/RTV)/H4_m \tag{22}$$

$$H7_{im} = \sum_k^{NG} q_k v_{ik} a_{km}/H4_m \tag{23}$$

The derived expression for entropy and enthalpy departures are:

$$\frac{S^R}{R} = -\frac{A^R}{RT} - \frac{b_T y_T}{b}\{\frac{4-2y}{(1-y)^3} + \frac{C(\alpha-1)[3 + 3\alpha y - (\alpha+1)y^2}{2(1-y)^3}\}$$

$$-(\frac{a_T b_T - ab_T - ab}{RTb^2}) \ln(1+4y) \tag{24}$$

and

$$\frac{H^R}{RT} = -Z - 1 - \frac{b_T y_T}{b}\{\frac{4-2y}{(1-y)^3} + \frac{C(\alpha-1)[3 + 3\alpha y - (\alpha+1)y^2]}{2(1-y)^3}$$

$$- \frac{4a}{RTb(1+4y)}\} - \frac{a}{Rb}(\frac{a_T}{a} - \frac{b_T}{b} - \frac{1}{T})\ln(1+4y) \tag{25}$$

where

$$b_T = \frac{db}{dT} \tag{26}$$

$$b_T = -\sum_i^{NC} X_i \sum_m^{NG} v_{im} b_m/T_m \tag{27}$$

$$a_T = (\partial a/\partial T)_{v,n} \tag{28}$$

$$a_T = Q^2 \sum_m^{NG} \sum_n^{NG} \theta_m \theta_n a_{nm} \tau_{nm}[\frac{\tau_{nm}^* - \tau_{nm}H4_m^*}{H4_m^2} + \frac{a_{nm}^* \tau_{nm}}{H4_m}] \tag{29}$$

$$a_{mn}^* = (da_{nm}/dT) \tag{30}$$

$$a_{mn}^* = -a_{mn}(\frac{1}{T_{mn}} + \frac{0.18135}{T}) \tag{31}$$

$$\tau_{mn}^* = (d\tau_{mn}/dT) \tag{32}$$

$$\tau_{mn}^* = (\frac{Q}{RTV}) \tau_{mn} \alpha_{mn} [(a_{mn}^* - a_{nn}^*) - \frac{a_{mn} - a_{nn}}{T}] \tag{33}$$

$$H4_m^* = \sum_k^{NG} \theta_k \tau_{kn}^* \tag{34}$$

OPTIMIZATION OF GROUP PARAMETERS

The MCORGC equation of state contains six parameters per group b_m^*, T_m^*, c_m, q_m, a_{mm}^* and T_{mm}^*. In addition, for each pair of groups three interaction parameters are needed, the attraction parameter a_{mn}^* and its characteristic temperature T_{mn}^* and the non random parameter α_{mn}. The group interaction parameters are assumed to be symmetrical; that is, $\alpha_{mn} = \alpha_{nm}$, $a_{mn} = a_{nm}$ and $T_{mn}^* = T_{nm}^*$.

In order to optimize group parameters, we followed the same procedure suggested by Moshfeghian and Maddox (1988) using a vapor liquid equilibrium data bank. The basic fitting procedure consisted of assembling the best available data for vapor pressure,

saturated vapor and liquid volumes, and heat of vaporization. These data were fitted simultaneously using a standard nonlinear analysis program. The predicted and experimental data for each set of parameters are then compared, and the summation of the error weighted squares is then minimized. The following objective function is used for pure component VLE data.

$$OF = \sum_{i}^{NP} \{W_1 (\frac{P_E^{sat} - P_C^{sat}}{P_E^{sat}})^2 + W_2 (\frac{V_E^v - V_C^v}{V_E^v})^2 + W_3 (\frac{V_E^l - V_C^l}{V_E^l})^2$$
$$+ W_4 (\frac{H_E^{vap} - H_C^{vap}}{H_E^{vap}})^2 \}_i \qquad (35)$$

where W_i's are the weighting factors for the relative errors of vapor pressure, vapor volume, liquid volume and heat of vaporization, respectively. In this study W_1 is set equal to 2 and W_2 through W_4 were set equal to 1. In the above equation P^{sat}, V^v, V^l and H^{vap} represent vapor pressure, vapor and liquid volumes and heat of vaporization, respectively. The subscripts

E and C stand for experimental and calculated values, respectively.

The optimized value of these parameters for 12 groups are presented in Table 1 and their binary group interactions in Table 2.

MODEL EVALUATION

In order to test the capability of the proposed model, thermodynamic properties of 28 oxygenated compounds including water have been predicted from a relatively low temperature up to the critical point. Figures 1 and 2 present the ability of MCORGC in predicting the pressure-volume diagram for methanol and ethanol. These are typical results obtained in this study. The vapor pressure predicted for several oxygenated compounds have been compared with the values reported in literature and shown in Figures 3 through 9. Saturated vapor volume is another vapor liquid equilibrium data that can be

TABLE 1. Oxygenated Group Parameters for MCORGC EOS (Zia-Razzaz and Moshfeghian, 1993)

No.	Group	b^*_m cm^3/mol	T_m, K	c_m	q_m	$a^*_{mm}/1000$ $cm^6\text{-}bar/moP$	T^*_{mm}, K
1	CH_3-	62.50	321.25	0.412	7.31	74.03	287.96
2	$-CH_2-$	43.40	973.40	1.024	4.66	80.23	472.62
3	$-CH<$	52.91	1340.00	-0.448	4.66	-167.10	268.03
3	$>CH<$	61.40	1823.80	-2.671	0.72	-28942.	303.84
4	MeOH	150.40	597.75	-13.084	12.40	268.40	366.33
5	$-OH (1°)$	50.30	612.12	1.357	10.34	606.45	131.27
6	$-OH (2°)$	68.99	205.83	10.996	10.34	243.99	230.81
7	$-OH (3°)$	61.38	419.69	1.292	10.34	817.37	110.69
8	CH_3-CO-	83.72	3042.60	10.195	12.83	113.42	841.81
9	$-CH_2-CO-$	75.02	1834.60	-6.472	10.45	91.30	502.74
10	CH_3-O-	57.44	1597.70	-2.014	9.38	130.42	208.17
11	$-O-$	45.62	7338.60	-4.925	6.72	157.68	189.49
12	H_2O	78.55	686.51	-14.399	12.07	132.62	528.26

TABLE 2. Binary Interaction Group Parameters for MCORGC EOS (Zia-Razzaz and Moshfeghian, 1993)

ψ_{IJ}	$a^*_{mn}/1000$ $cm^6\text{-}bar/mol^2$	T^*_{mn}, K	a^*_{mn}, K
102	57.678	626.26	0.000
103	49.946	746.90	0.000
104	246.910	1074.40	0.000
105	156.880	371.31	-0.235
106	129.870	285.42	0.299
107	150.600	277.56	-0.228
108	82.724	586.04	-0.294
109	63.664	726.27	-0.991
110	105.710	577.53	-0.689
111	114.530	492.00	-1.120
203	145.500	185.78	0.000
205	95.712	466.61	-1.020
208	25.549	1860.80	24.210
209	32.853	974.49	6.221
210	51.516	2049.70	-4.047
211	82.642	364.44	-15.020
306	49.946	328.98	1.309
307	524.420	265.91	-0.070

$\psi_{IJ} = 100.$ (Group No. I) + (Group No. J)

calculated by an EOS. Typical ability of MCORGC in predicting the saturated vapor volume is shown in
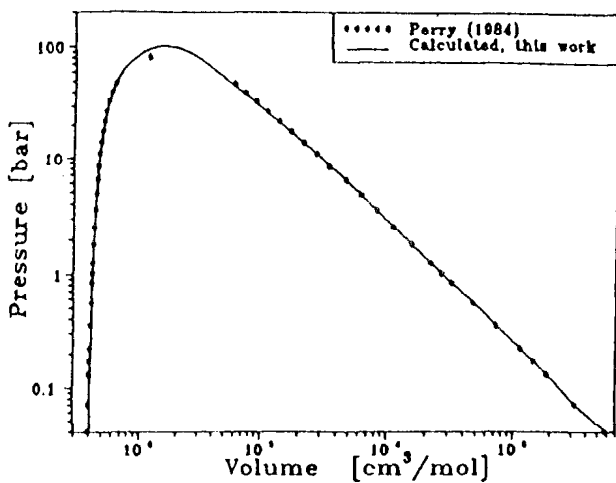

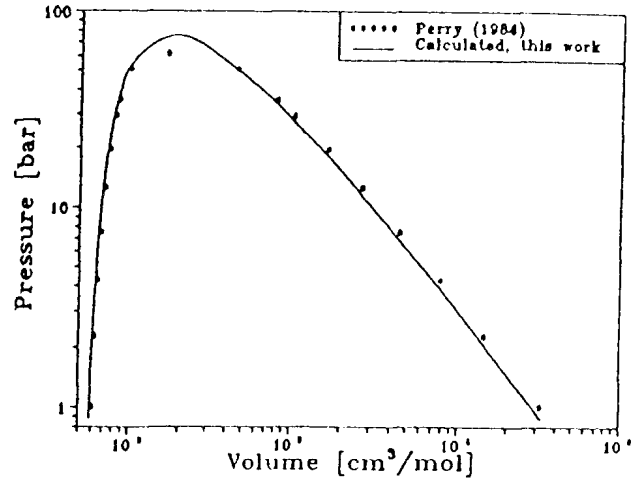Figure 1. Coexistence volumes for Methanol.

Figure 2. Coexistence volumes for Ethanol.

Figures 10 and 11 for iso-propanol and tertiary butanol. The results of saturated liquid densities calculated for a number of compounds are shown in Figures 12 and 13. At this moment, no equation of state is known with the same capability of predicting liquid densities. Latent heat of a pure compound can be calculated by subtracting coexistence vapor and liquid residual enthalpies. Latent heats of several compounds have been calculated and shown in Figures 14 through 15.

The predicted properties have been compared with the values reported in literature and the results of this comparison are also reported in Table 3. Unfortunately, for all compounds tested, all of the required thermodynamic
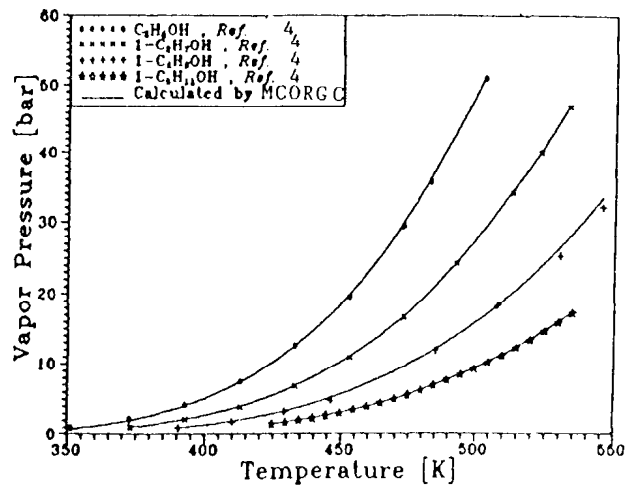

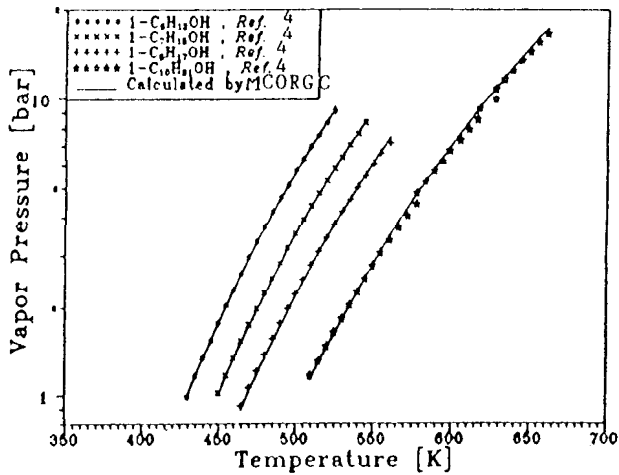
Figure 3. Vapor pressure of 1° Alcohols (I).
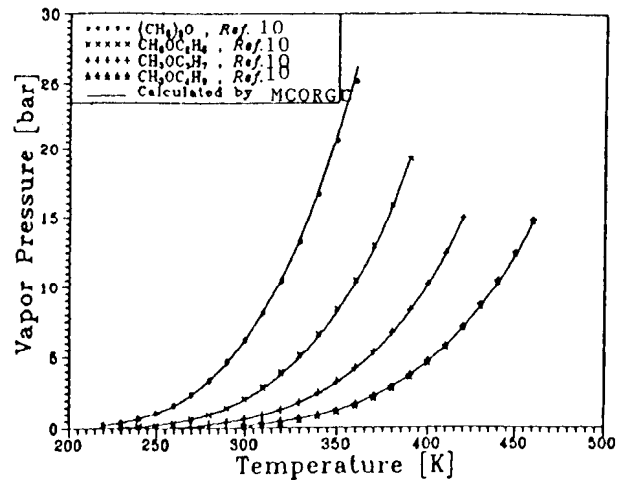
Figure 4. Vapor Pressure of 1° Alcohols (II).

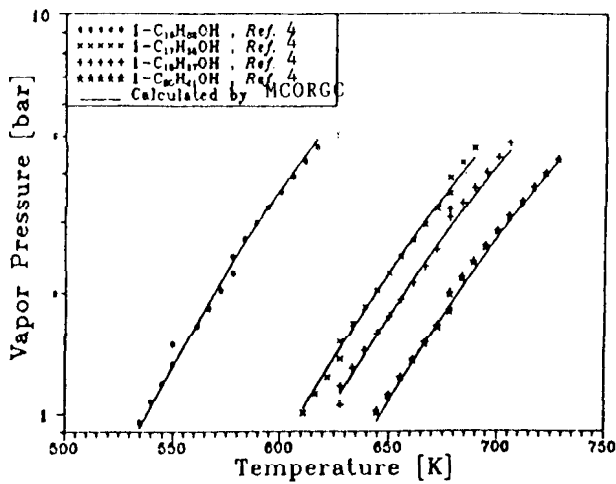**Figure 7.** Vapor pressure of Ethers (I).

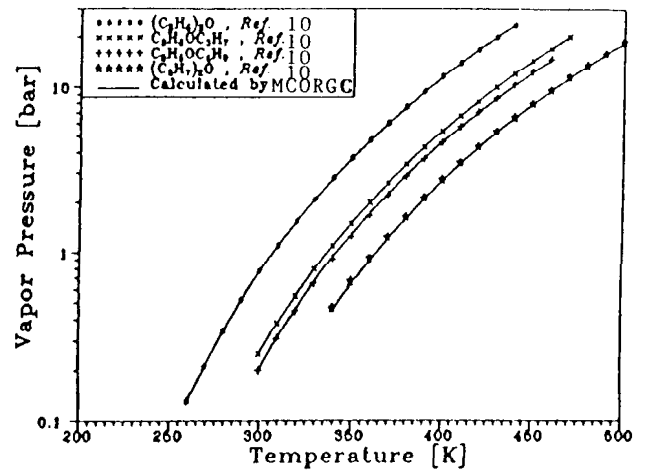**Figure 5.** Vapor pressure of 1° Alcohols (III).

Figure 8. Vapor pressure of Ethers (II).
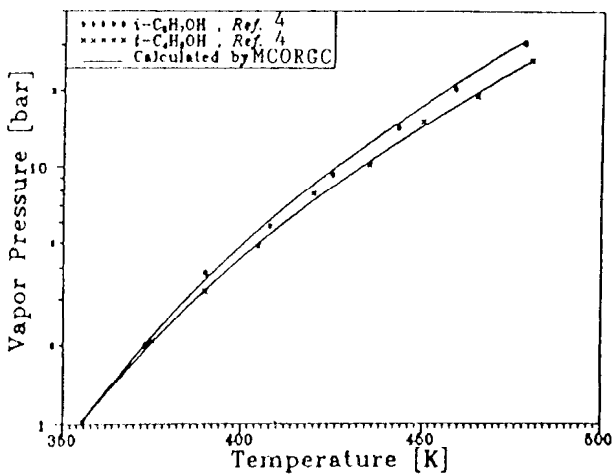
Figure 6. Vapor pressure of 2° & 3° Alcohols.

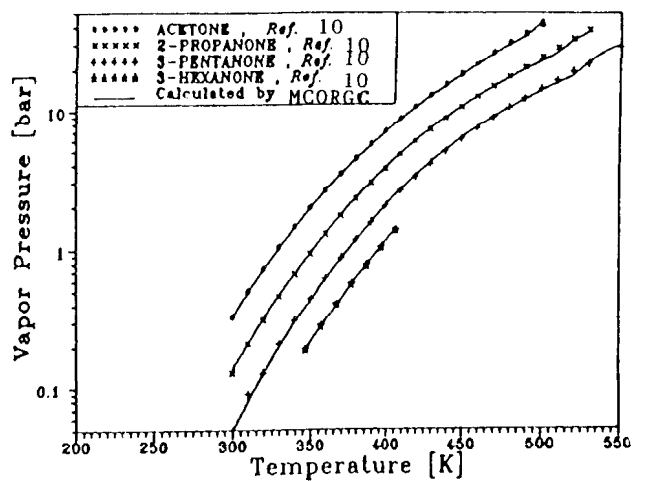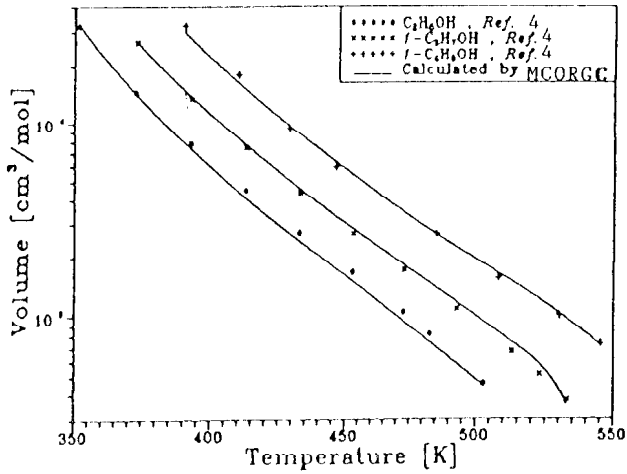**Figure 9.** Vapor pressure of Ketones.

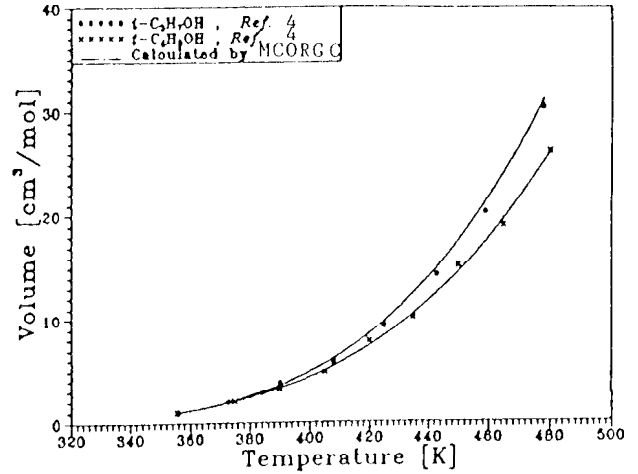**Figure 10.** Saturated vapor volumes of 1° Alcohols.

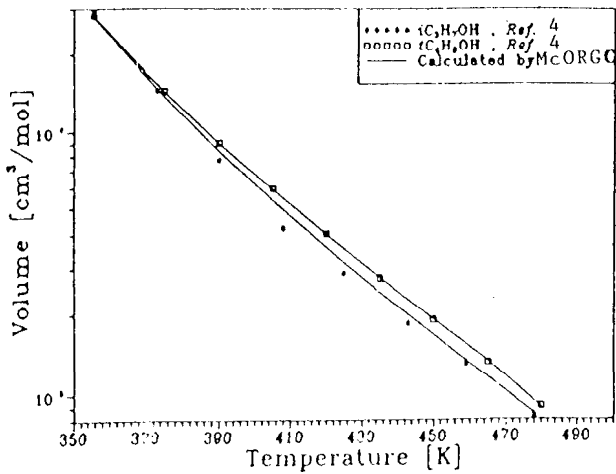**Figure 13.** Saturated liquid volumes of 2° & 3° Alcohols.

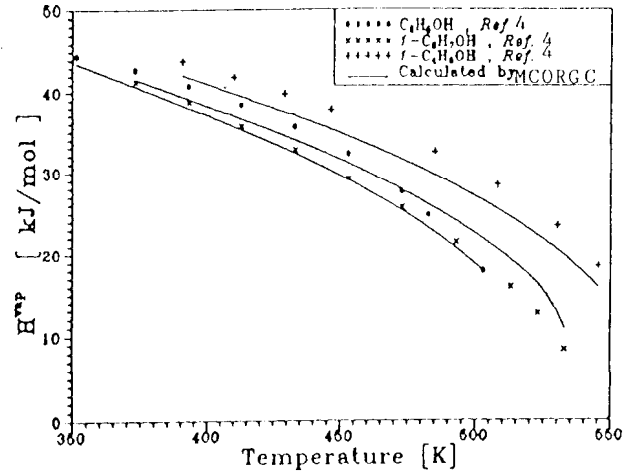**Figure 11.** Saturated vapor volumes of 2° & 3° Alcohols.
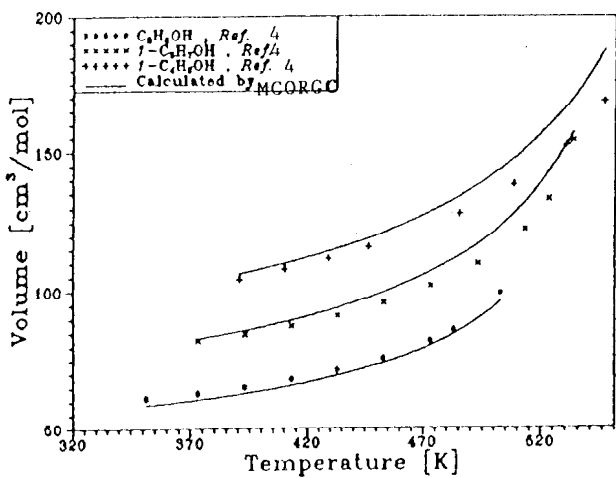

Figure 14. Heat of vaporization of 1° Alcohols.

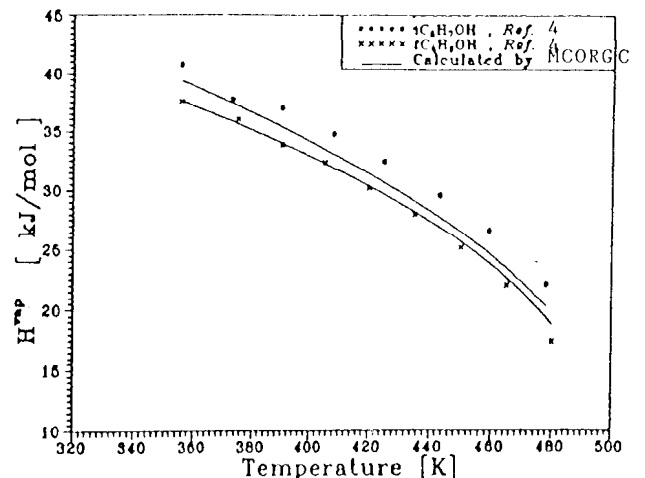**Figure 12.** Saturated liquid volumes of 1° Alcohols.

Figure 15. Heats of vaporization of 2° & 3° Alcohols.

TABLE 3. Accuracy of MCORGC in Predicting the Saturated Properties of Oxygeneated Compounds

Substance	No. of Points	Ref. No.	Temp. Range, K	T_r Range	Average absolute percent deviation			
					P	V^v	V^l	H^{vap}
water	51	1	339-617	0.52-095	1.70	3.63	2.25	2.98
methanol	24	5	273-484	0.53-0.94	1.68	1.17	0.91	5.37
ethanol	9	5	351-503	0.68-0.97	3.51	6.69	2.93	6.77
propanol	10	4	371-533	0.70-0.99	1.38	5.87	4.11	9.03
1-butanol	8	4	390-546	0.69-0.97	4.21	4.71	5.19	8.99
1-pentanol	23	4	425-535	0.72-0.91	0.67	—	—	—
1-hexanol	20	4	430-525	0.70-0.86	0.50	—	—	—
1-heptanol	20	4	450-545	0.71-0.86	0.94	—	—	—
1-octanol	20	4	465-561	0.71-0.86	1.83	—	—	—
1-decanol	31	4	510-661	0.76-0.98	2.99	—	—	—
1-dodecanol	17	4	535-616	0.79-0.91	3.43	—	—	—
1-heptadecanol	17	4	611-689	0.83-0.94	3.18	—	—	—
1-octadecanol	17	4	628-706	0.84-0.94	3.87	—	—	—
1-eicosanol	17	4	644-728	0.84-0.94	3.05	—	—	—
2-propanol	8	4	355-478	0.70-0.94	3.89	6.83	1.91	5.05
t-butanol	9	4	355-480	0.70-0.95	2.72	0.33	0.27	1.70
acetone	21	10	300-500	0.59-0.98	1.42	—	—	—
2-butanone	24	10	300-530	0.56-0.99	1.67	—	—	—
3-pentanone	18	10	330-500	0.60-0.91	1.06	—	—	—
3-hexanone	7	10	347-407	0.60-0.70	1.42	—	—	—
dimethyl ethter	15	10	220-360	0.55-0.90	1.58	—	—	—
methyl ethyl ether	17	10	230-390	0.52-0.89	2.64	—	—	—
diethyl ether	19	10	260-440	0.56-0.94	0.38	—	—	—
methyl propyl ether	17	10	260-420	0.55-0.88	2.31	—	—	—
ethyl propyl ether	18	10	300-470	0.60-0.94	0.49	—	—	—
methyl buthyl ether	17	10	300-460	0.58-0.90	1.53	—	—	—
dipropyl ether	17	10	340-500	0.64-0.94	2.31	—	—	—
ethyl butyl ether	17	10	400-500	0.64-0.94	1.96	—	—	—
Average AAD%					**2.08**	**4.17**	**2.51**	**5.69**

properties were not available to make a full comparison. As can be seen from Table 3, the average absolute deviation for vapor pressure is 2.08%. The average absolute deviations for other properties (for 7 pure compounds) are 4.17% for saturated vapor volume, only 2.51% for saturated liquid volume (liquid density), and 5.69% for latent heat. Considering the non ideality of systems considered, the accuracies obtained are within the satisfactory range. The calculated properties are usually as accurate as experimental values themselves and the order of errors (specially for

liquid density) is very low.

COMPARISON WITH OTHER EOS

The saturation state properties of a number of compounds have been calculated using different versions of the CORGC equation of state. The comparison results in terms of average absolute deviation are shown in Table 4 through 7. As can be seen, almost all predictions of the proposed MCORGC are much more accurate than those of the others.

equation of state, MCORGC, based on the CORGC and a NRTL type local composition mixing rule applicable to oxygenated compounds have been evaluated and the results of this evaluation are presented. Its ability to predict the thermodynamics properties of pure components systems, tested against reported experimental data, have led to a reasonable degree of agreement. In addition, its ability and accuracy, compared with other equations of state, produced superior results.

Work is underway to extended this study to multicomponent non ideal systems.

CONCLUSIONS

Capabilities and accuracy of a new group contribution

TABLE 4. Comparison between Different Versions of CORGC in Predicting Vapor Pressure of Alcohols

Substance	T_r Range	Average absolute percent deviation		
		Pults (1988)	Shariat et al. (1993)	MCORGC
methanol	0.53-0.94	———	1.94	1.68
ethanol	0.68-0.97	5.16	7.43	3.51
propanol	0.70-0.99	4.60	3.19	1.38
1-butanol	0.69-0.97	4.00	4.00	4.21
1-pentanol	0.72-0.91	0.74	3.53	0.67
1-hexanol	0.70-0.86	2.04	4.92	0.50
1-heptanol	0.71-0.86	———	4.98	0.94
1-octanol	0.71-0.86	5.19	5.78	1.83
1-decanol	0.76-0.98	2.04	5.54	2.98
1-dodecanol	0.79-0.91	3.54	5.65	3.43
1-heptadecanol	0.83-0.94	———	7.53	3.18
1-octadecanol	0.84-0.94	9.34	10.24	3.87
1-eicosanol	0.84-0.94	———	11.97	3.05
Average (1) AAD%		———	5.90	2.04
Average (2) AAD%		4.07	5.59	2.48

(1) Average for all listed compounds

(2) Average for compounds listed by Pults (1988)

TABLE 5. Comparison between Different Versions of CORGC in Predicting Vapor Volume of Alcohols

Substance	T_r Range	Average absolute percent deviation		
		Pults (1988)	Shariat et. al. (1993)	MCORGC
methanol	0.53-0.94	——	1.16	1.17
ethanol	0.68-0.97	——	1.90	6.68
propanol	0.70-0.99	——	13.40	5.87
1-butanol	0.69-0.97	——	5.49	4.71
Average AAD%			**5.49**	**4.61**

TABLE 6. Comparison between Different Versions of CORGC in Predicting Liquid Volume of Alcohols

Substance	T_r Range	Average absolute percent deviation		
		Pults (1988)	Shariat et. al. (1993)	MCORGC
methanol	0.53-0.94	——	0.43	0.91
ethanol	0.68-0.97	11.30	3.26	2.83
propanol	0.70-0.99	4.53	2.85	4.11
1-butanol	0.69-0.97	1.59	4.59	5.19
Average (1) AAD%		——	**2.78**	**3.26**
Average (2) AAD%		**5.81**	**3.57**	**4.04**

(1) Average for all listed compounds
(2) Average for compounds listed by Pults (1988)

TABLE 7. Comparison between Different Versions of CORGC in Predicting Latent Heat of Alcohols

Substance	T_r Range	Average absolute percent deviation		
		Pults (1988)	Shariat et. al. (1993)	MCORGC
methanol	0.53-0.94	——	4.42	5.37
ethanol	0.68-0.97	——	8.82	6.77
propanol	0.70-0.99	——	13.74	9.02
1-butanol	0.69-0.97	——	5.88	8.99
Average AAD%		——	**8.21**	**7.54**

LIST OF SYMBOLS

a	attraction energy parameter of an EOS, (cm^6. bar/mol^2)
a'	$(\partial a/\partial V)$, ($cm^5/mol^2/K$)
a_{mn}	attraction energy between groups m and n, (cm^6. $bar/mol/K$)
a_T	$(\partial a/\partial T)$, ($cm^6.bar/mol^2/K^2$)
b	covolume (cm^3/mol)
b_i	covolume of molecule i (cm^3/mol)
b_m	covolume of group m, ($cm^3.bar/mol$)
b_T	$(\partial b/\partial T)$, ($cm^3/mol/K$)
C	equivalent degree of freedom
c_i	equivalent degree of freedom of molecule i
c_m	equivalent degree of freedom of group m
$H2_m, H3_m,...$	auxiliary parameters of the modified CORGC equation
H^R	residual enthalpy, (J/mol)
H^{vap}	vaporization enthalpy, (KJ/mol)
n	number of moles, (mol)
NC	number of components
NG	number of groups
NP	number of data point
P	pressure (bar)
P^{sat}	saturated pressure, (bar)
Q	normalized molecular surface area of fluid
q_i	normalized molecular surface area of molecule i
q_m	normalized surface area of group m
R	universal gas constant, 83.14 ($cm^3.bar/mol/K$)
S^R	residual entropy, (J/mol/K)
T	temperature (K)

T_m	covolume parameter temperature dependency, (K)
T^*_{mn}	energy parameter temperature dependency, (K)
V	volume (cm³/mol)
V^l	liquid volume (cm³/mol)
V^v	vapor volume (cm³/mol)
X_i	liquid mole fraction of component i
Y_i	vapor mole fraction of component i
y	b/4V, dimensionless density
Z	compressibility coefficient
W_1, W_2, W_3, W_4	weighting factors for the error objective functions
α	dumbbell geometric constant 1.037
α_{mn}	non randomness parameter
τ_{ii}	local composition parameter
ϕ	fugacity coefficient
V_{im}	number of group m in the molecule i
θ_m	area fraction of group m

Subscript	Description
C	critical point properties
m	group properties of group m
n	group properties of group n
i	molecular properties of component i
r	reduced property
T	derivation with respect to temperature

Superscript	Description
l	liquid properties
R	residual properties
v	vapor properties

Abbreviation	Description
AAD	average absolute deviation
AAD%	average absolute deviation percent
EOS	equation of state
GC-EOS	group contribution equation of state
i-	branched molecule

n-	normal (straight-chain) molecule
NRTL	non-random two liquid theory
PFGC	parameters from group contribution

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